

Data dictionary for U.S.EPA ScienceHub dataset “*The Acute Toxicity of Major Ion Salts to Ceriodaphnia dubia: II. Empirical Relationships in Binary Salt Mixtures*” (short name “MED Ion Tox Paper2”). This dataset is contained in the zip file “MEDIonToxPaper2_Dataset.zip”, consisting of the following files:

I. 29 csv files named TDS-yy-*nn*.csv providing biological results and general chemistry for different experiments, with the following organization and format:

A. Each file describes a single experiment consisting of 6-7 binary mixture tests regarding the acute toxicity of major ion salts to *Ceriodaphnia dubia*.

B. Each file starts with several header rows with general experimental information.

C. Each file then has several blocks of information, each block providing data for one toxicity test.

D. Each block of information consists of 1-2 header rows with general test information, 2 rows of headings for data columns, 20 rows providing data for each test unit, 0-2 footnote rows, and 2 blank rows separating it from the next block.

E. Each data row provides the following information for a test replicate:

1. The treatment concentration as a percentage of the highest concentration
2. The replicate identification
3. Concentration of chemical A (mg/L)
4. Concentration of chemical B (mg/L)
5. The initial number of test organisms
6. The number of surviving test organisms at 24 hours
7. The number of surviving test organisms at 48 hours
8. Hardness mg/L as CaCO₃. at test start
9. Alkalinity mg/L as CaCO₃. at test start
10. pH at test start
11. Dissolved Oxygen mg/L. at test start
12. Conductivity ms/cm. at test start
13. Dissolved Oxygen mg/L. at test end
14. Alkalinity mg/L as CaCO₃. at test end (data only for a few tests)

15. pH at test end
16. Conductivity ms/cm. at test end
17. Temperature at test end

II. “*MEDIonToxPaper2_SupplementalDataFinal2*” in .csv, .xlsx, and pdf formats, providing the following information regarding the median lethal conditions for each toxicity test:

1. Experiment ID in TDS-yy-*nn*
2. Test chemical A identity
3. Test chemical A added concentration in median lethal mixture (LC50A)
4. Lower confidence limit for LC50A
5. Upper confidence limit for LC50A
6. Test chemical B identity
7. Test chemical B added concentration in median lethal mixture (LC50B)
8. Lower confidence limit for LC50B
9. Upper confidence limit for LC50B
10. Total Na Concentration (mM) at LC50
11. Total K Concentration (mM) at LC50
12. Total Ca Concentration (mM) at LC50
13. Total Mg Concentration (mM) at LC50
14. Total Cl Concentration (mM) at LC50
15. Total SO₄ Concentration (mM) at LC50
16. Alkalinity (meq/L) at LC50
17. pH at LC50
18. Ca⁺² Activity at LC50
19. Mg⁺² Activity at LC50
20. Na⁺ Activity at LC50
21. K⁺ Activity at LC50
22. Cl⁻ Activity at LC50
23. SO₄⁻² Activity at LC50
24. CO₃⁻² Activity at LC50
25. HCO₃⁻ Activity at LC50
26. H₂CO₃* Activity at LC50
27. Nominal Osmolarity (mOsm/L) at LC50
28. Estimated Osmolarity (mOsm/L) at LC50